Minimal Stencil Finite Volume Scheme with the Discrete Maximum Principle

**Konstantin Lipnikov,
Daniil Svyatskiy, T-5;
Yuri Vassilevki, Russian
Academy of Sciences (RAS)**

The maximum (or minimum) principle is an important property of linear and nonlinear advection-diffusion type problems. It is very desirable to mimic this property in numerical simulations in a wide range of applications. Violation of the discrete maximum principle (DMP) leads to non-physical solutions with numerical artifacts, such as a heat flow from a cold material to a hot one. These oscillations can be significantly amplified by the non-linearity of the physics. Unfortunately, numerical schemes that satisfy the DMP impose severe limitations on mesh geometry and problem coefficients. We developed a new nonlinear finite volume method that guarantees the DMP for numerical solutions on general polygonal meshes for diffusion-advection problems with anisotropic coefficients.

The diffusion-type problem can be written in the divergence form as follows:

$$\mathrm{div}\,\mathbf{q}=f \quad \text{and} \quad \mathbf{q}= -\mathbb{K}\nabla c + v_c$$

where $\mathbb{K}(\mathbf{x})$ is a symmetric positive definite continuous (possibly anisotropic) diffusion tensor, v is a velocity, f is a source term and $c(x)$ is an unknown scalar function, for example concentration. The vector function $\mathbf{q}(x)$ is an unknown concentration flux. The first equation represents the mass conservation law. The second is the constitutive equation that establishes connection between scalar and vector unknowns. In subsurface modeling, this law is referred to as Darcy's law–similar laws go by different names in other areas. An appropriate boundary condition should be imposed to make the problem well posed.

State-of-art second order discretization schemes, such as the Mixed Finite Element (MFE) method, Mimetic Finite Difference (MFD) method, and Multi-Point Flux Approximation (MPFA) method, fail to provide a solution that satisfies the discrete maximum principle or even to preserve positivity of a numerical solution when the diffusion tensor is heterogeneous and anisotropic or the computational mesh is strongly perturbed.

The finite volume framework has several obvious advantages. It operates with cell-centered degrees of freedom (minimum number of unknowns) and provides the local mass conservation by construction because the equation is discretized in the mixed form. The classical *linear* two-point (FV) scheme defines a flux across a mesh edge as the difference between two concentrations at neighboring cells multiplied by a transmissibility coefficient. It results in a linear system of equations with a matrix that has special properties (M-matrix with diagonal dominance in rows). This immediately implies the discrete maximum principle. These properties along with the minimal discretization stencil (number of non-zero entries in each matrix row) make this approach very popular in many modeling tools and legacy codes. However, the accuracy of this scheme depends on the mesh geometry, mutual orientation of the mesh edges, and principal directions of the diffusion tensor. More precisely, to provide minimal order of accuracy the principal directions have to be orthogonal to the mesh edges, which is clearly an impossible requirement for arbitrary tensors and/or arbitrary polygonal cells. The MPFA scheme solves the accuracy problem by using more than two points in the flux stencil and a matrix of transmissibility coefficients. This makes the discretization stencil larger. The MPFA scheme provides a second-order accurate approximation, but is often only conditionally stable and conditionally monotone.

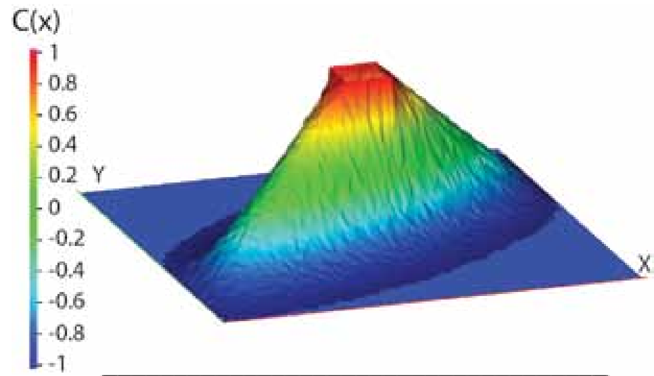
To incorporate the monotonicity requirement into the finite volume framework, we use the ideas propsed by E. Bertolazzi, [1] along with the fact that coefficients in flux discretization depend on the unknowns in neighboring cells even for liinear diffusion-advection problems. Several approaches based on this idea have been proposed recently, but all of them guarantee only positivity preservation of a numerical solution on general meshes for general tensor coefficients. To guarantee the DMP, a *nonlinear* multi-point approximation of the flux is essential. For diffusion problems, a new method was proposed that uses multi-point approximation of the flux along with interpolation techniques and auxiliary unknowns at the mesh vertices [3]. The use of interpolation techniques and auxiliary unknowns increases the stencil and makes it difficult to incorporate this approach into existing modeling tools. In our research, we propose an interpolation-free multi-point nonlinear approximation of diffusive fluxes. The proposed scheme has the minimal stencil and reduces to the classical two-point FV scheme on Voronoi or rectangular meshes for scalar (and, in a few cases, diagonal tensor) coefficients.

For more information contact Daniil Svyataskiy at dasvyat@lanl.gov.

Funding Acknowledgments
DOE, Office of Science, Advanced Scientific Computing Research Program in Applied Mathematics

The resulting nonlinear algebraic system is sparse, but non-symmetric. For quadrilateral meshes there are at most four non-zero elements in each row. We elaborated on this system and proved, theoretically as well as demonstrating in the numerical tests (see Fig. 1), that the numerical solution satisfies the DMP principle. Moreover, if the nonlinear system is solved using the Picard iterative method then the proposed method guarantees that the DMP is satisfied on all iterative steps. It means that for any tolerance of the iterative method we obtain a monotone solution. The proof is based on the special properties of M-matrices.

The numerical experiments presented in [2] also study this approach for advection-diffusion problems and demonstrate its monotone properties and accuracy. The method can be applied on unstructured polygonal meshes and full anisotropic heterogeneous diffusion tensors. The second-order convergence is observed for scalar unknowns C_h. For numerical approximation q_h, of the normal components of the flux q the convergence rate, is higher than the first order.



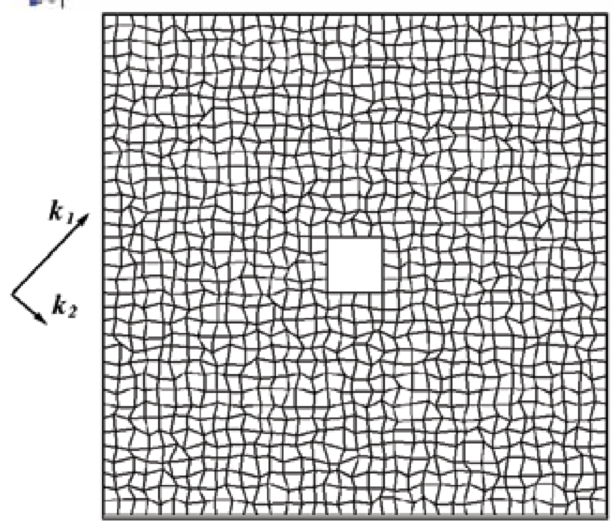


Fig. 1. (Top): Profile of numerical solution $C_h(x,y)$ on the distorted quadrilateral mesh, $-1 \le C_h(x,y,) \le 1$. (Bottom): Computational domain for the anisotropic diffusion problem: The unit square with the hole in the center. The problem becomes the diffusion equation with highly anisotropic tensor. Ratio of tensor's eigenvalues is 10^3. Tensor is rotated with respect to coordinate axes on 60° clockwise. $C_h=1$ on the hole, $C_h=-1$ on the boundary of unit square. Analytical solution satisfies maximum principle, $-1 \le c(x,y,) \le 1$.

[1] Bertolazzi, E. *Math. Mod. Meth. Appl. S.,* **8**,(4), 685 (1998).

[2] Sheng, Z. and G. Yuan, *.J Comput Phys* **230**(7), 2588 (2011).

[3] Lipnikov, K. et al., *Russ. J. Numer. Anal. Math. Modelling,* 27(4), 369 (2012).